

# Thermodynamical properties of a trapped interacting Bose gas

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The thermodynamical properties of interacting Bose atoms in a harmonic potential are studied within the mean-field approximation. For weak interactions, the quantum statistics is equivalent to an ideal gas in an effective mean-field potential. The eigenvalue of the Gross-Pitaevskii equation is identified as the chemical potential of the ideal gas. The condensation temperature and density profile of atoms are calculated. It is found that the critical temperature  $T_c$  decreases as the interactions increase. Below the critical point, the condensation fraction exhibits a universal relation of  $N_0/N = 1 - (T/T_c)^\gamma$ , with the index  $\gamma \approx 2.3$  independent of the interaction strength, the chemical potential, as well as the frequency of the confining potential.

Keywords: interacting boson; mean-field approximation; condensation temperature

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## I. INTRODUCTION

Since the first observations of the Bose-Einstein condensation (BEC) in dilute alkali-metal atom gases[1–3], experimental developments have posed many new tests for many-body theory. Numerous theoretical approaches have been implemented in order to obtain accurate results for both the ground-state and non-equilibrium properties of the trapped boson systems[4–7]. Although there is a vast number of studies in literature, the effects of interactions on the transition temperature of BEC still remains an open question. The current consensus among physicists is that the interaction-caused shift in condensation temperature  $\Delta T_c \equiv T_c^{(a)} - T_c^{(0)}$ , where  $T_c^{(0)}$  and  $T_c^{(a)}$  are respectively the critical temperature for ideal and interacting gases, satisfies a linear relation  $\Delta T_c/T_c^{(0)} \approx c a_s n^{1/3}$  with respect to the  $s$ -wave scattering length  $a_s$ . Here  $n$  is the particle density. However, the value and even the sign of the coefficient  $c$  is controversial[8]. Some authors claimed that repulsive interactions reduce the critical temperature[9–12], while others indicated an increase of the critical temperature[13–21]. In a recent publication[22], the authors obtained a negative constant  $c \approx -2.33$  by using the model of spatial permutations. This contradiction is somehow reconciled by a recent experiment[23], where the researchers demonstrated a negative shift of the critical temperature for weak interactions and a positive shift for sufficiently strong interactions.

For an ideal Bose gas in a harmonic trap  $V(\mathbf{r}) = \frac{1}{2}m\omega^2 r^2$ , the BEC temperature  $T_c$  is determined by  $k_B T_c = \hbar\omega(N/\zeta(3))^{1/3}$ , with  $\zeta(3) = 1.202$ [6, 7, 24]. The fraction of condensation at a temperature  $T$  below  $T_c$  is  $N_0/N = 1 - (T/T_c)^3$ , where  $N_0$  is the number of Bose particles in the condensed state. In this paper, we explore the phase transition properties of interacting Bose atoms confined in a spherically symmetric harmonic

potential within the mean-field approximation (MFA). We show that in the weak interaction limit the particle distribution is equivalent to the ideal gas in an effective mean-field potential. The eigenvalue of the generalized Gross-Pitaevskii (GP) equation is identified as the chemical potential of the ideal gas. For the condensed atoms we obtain the density profile within the Thomas-Fermi approximation. The condensation temperature  $T_c$  decreases with increase of interactions as  $T_c \sim a_s^{-\beta}$  with  $\beta \approx -0.75$ , in contrast to the previous mean-field calculations which gave a linear relation  $\Delta T_c/T_c^{(0)} \approx -2.47 a_s n^{1/3}$ [12, 23]. Our results qualitatively coincide with the recent measurement[23]. In particular, the  $T_c$  is independent of confining frequency which implies the details of the external potential is unimportant to the BEC. Below the critical temperature, we find a universal relation between the condensed fraction and the temperature  $N_0/N = 1 - (T/T_c)^\gamma$ , with an index  $\gamma \approx 2.3$  being independent of the interaction strength, the chemical potential, as well as the frequency of the confining potential.

The paper is organized as following: In Sec.II we briefly introduce the mean-field theory and the related results. Section III displays our main numerical results. A brief summary is included in Sec.IV.

## II. MEAN-FIELD THEORY

The Hamiltonian for an interacting Bose gas in a external trap  $V(\mathbf{r})$  is

$$\hat{H} = \int d\mathbf{r} \{\hat{\psi}^\dagger [-\frac{\hbar^2}{2m} \nabla^2 + V] \hat{\psi} + \frac{g}{2} |\hat{\psi}|^4\}, \quad (1)$$

where the coupling constant  $g = 4\pi\hbar^2 a_s/m$  is written in terms of the scattering length  $a_s$  and atom mass  $m$ . Following the standard approach, the Bose field operator is decomposed as  $\hat{\psi} = \Phi + \hat{\phi}$ , where  $\Phi$  is a  $c$ -number for the condensate, and  $\hat{\phi}(\mathbf{r})$  is an operator representing its fluctuations which annihilates a thermal atom at  $\mathbf{r}$ .

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Excluding the possibility of aggregate motion and vortices, the stationary state of  $\Phi(\mathbf{r})$  satisfies the generalized GP equation[25–27]

$$-\frac{\hbar^2}{2m} \nabla^2 \Phi + [V(\mathbf{r}) - \mu + g(n_0(\mathbf{r}) + 2n_T(\mathbf{r}))]\Phi = 0, \quad (2)$$

where  $\mu$  is the eigenvalue of the GP equation. The equation of motion for  $\langle\phi(\mathbf{r}, t)\rangle$  is

$$i\hbar \frac{\partial \langle\hat{\phi}\rangle}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \langle\hat{\phi}\rangle + [V(\mathbf{r}) - \mu + 2gn(\mathbf{r})]\langle\hat{\phi}\rangle + gn_0(\mathbf{r})\langle\hat{\phi}^\dagger\rangle. \quad (3)$$

The condensate density and the number of condensate atoms are defined by  $n_0(\mathbf{r}) = |\Phi(\mathbf{r})|^2$  and  $N_0 = \int d\mathbf{r} n_0(\mathbf{r})$ , respectively. The noncondensate (thermal) density is  $n_T = \langle\hat{\phi}^\dagger\hat{\phi}\rangle$ , where  $\langle\cdots\rangle$  indicates a thermal average in the grand-canonical ensemble. The generalized nonlinear GP equation (2), which includes interactions between the condensate and the thermal atoms, is solved for a static condensate, while the quasiparticle excitations of the system is described by the coupled Bogoliubov equations (3), which yields the quasiparticle energies and amplitudes. These in turn determine the number of noncondensed atoms  $N_T$  as well as various coherence terms thermodynamic averages over two or more Bose field operators.

As emphasized in Ref.[28], the coherence terms  $m_T = \langle\hat{\phi}\hat{\phi}\rangle - \Phi^2$  yield an excitation spectrum that is not gapless. The Popov approximation, which neglects these terms, reduces the third and fourth-order terms in  $\hat{\phi}$  and  $\hat{\phi}^\dagger$ , respectively, to the first and second order so that the Hamiltonian can be diagonalized[29]. Although it has been successful in describing the properties of the trapped Bose gases, it is not well-grounded theoretically, and fails to yield accurate predictions for the low-lying excitations at high temperatures.

The elementary excitations in Eq.(3) can be obtained by employing the semiclassical WKB approximation[12]. The coupled equations for  $\langle\hat{\phi}\rangle$  and its complex conjugate  $\langle\hat{\phi}^\dagger\rangle$ , can be solved explicitly, and the semiclassical excitation spectrum is obtained as

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$$\epsilon(\mathbf{p}, \mathbf{r}) = \sqrt{\left[\frac{p^2}{2m} + V(\mathbf{r}) - \mu + 2gn(\mathbf{r})\right]^2 - g^2 n_0^2(\mathbf{r})}. \quad (4)$$

For a homogeneous system at low temperatures,  $n_T$  can be neglected, and the above excitations coincide with the usual Bogoliubov spectrum.

The quasiparticles with energies  $\epsilon(\mathbf{p}, \mathbf{r})$  are distributed according to the Bose distribution function,

$$f(\mathbf{p}, \mathbf{r}) = \{\exp[\beta\epsilon(\mathbf{p}, \mathbf{r})] - 1\}^{-1}, \quad (5)$$

where  $\beta = 1/k_B T$ . The particle distribution function can be obtained from the Bogoliubov canonical transformations and is given by

$$F(\mathbf{p}, \mathbf{r}) = -\left(\frac{\partial\epsilon}{\partial\mu}\right)_{n_0} f(\mathbf{p}, \mathbf{r}). \quad (6)$$

It is notable that the identification of the chemical potential  $\tilde{\mu}$  with the eigenvalue  $\mu$  of the GP equation is questionable in general. In the grand-canonical ensemble, the chemical potential is defined as  $\tilde{\mu} = \partial E / \partial N$ , corresponding to the energy cost  $E$  of adding a particle to the entire system, not only to the condensate. However, in the framework of the present theory, the excitation energies (4) can be approximately reduced to the first order of coupling strength  $g$  as

$$\epsilon(\mathbf{p}, \mathbf{r}) \approx \frac{p^2}{2m} + V(\mathbf{r}) - \mu + 2gn(\mathbf{r}). \quad (7)$$

Therefore,  $(\partial\epsilon/\partial\mu)_n \approx -1$ , yielding the thermal density distribution

$$n_T(\mathbf{r}) \approx \int \frac{1}{\exp[\beta(p^2/2m + V_{eff}(\mathbf{r}) - \mu)] - 1} \frac{d\mathbf{p}}{(2\pi\hbar)^3}, \quad (8)$$

This equation is exactly equivalent to the statistics of an ideal Bose gas confined in an effective mean-field potential,

$$V_{eff} = V(\mathbf{r}) + 2gn(\mathbf{r}). \quad (9)$$

Consequently, the eigenvalue  $\mu$  of the GP equation (2) is justified as the chemical potential of the ideal gas in the effective potential.

The result can be understood as following: Suppose an interacting Bose gas is trapped in an external potential  $V(\mathbf{r})$  which reaches an equilibrium distribution  $n(\mathbf{r})$ . Adding an extra noninteracting Bose atom increases an energy  $\Delta\epsilon(\mathbf{r}) = V(\mathbf{r}) + 2gn(\mathbf{r})$ . As the new comer is assimilated into the interacting gas, the density distribution  $n(\mathbf{r})$  adjust slightly in order to transfer the increased energy into the effective potential. The factor 2 in the effective potential (9) comes from the Bose symmetry.

### III. NUMERICAL RESULTS

At finite temperature  $T$  below  $T_c$ , interaction effects involving the thermal atoms should be taken into account in addition to those of the condensate, especially when  $T$  goes close to  $T_c$ . Integrating over the momentum  $\mathbf{p}$  in Eq.(8), we obtain in the harmonic potential,

$$n_T(\mathbf{r}) = \sum_{k=1}^{\infty} \frac{e^{-k\beta(m\omega^2 r^2/2 + 2gn(\mathbf{r}) - \mu)}}{(\lambda_T \sqrt{k})^3}, \quad (10)$$

where  $\lambda_T = (2\pi\hbar^2/mk_B T)^{1/2}$  is the thermal de Broglie wavelength.

From the generalized GP equation (2), the Thomas-Fermi approximation

$$\mu = V(\mathbf{r}) + g[n_0(\mathbf{r}) + 2n_T(\mathbf{r})], \quad (11)$$

will be used in the following discussions. For a spherically symmetric potential, there is a boundary radius  $r_1$ . For

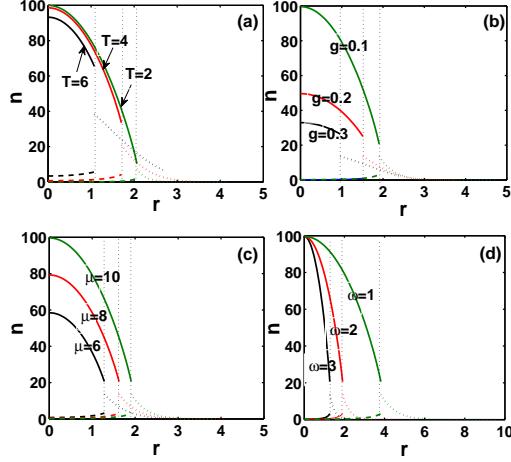


FIG. 1: (Color online) Density distributions of the condensed (real curves) and noncondensed (dashed and dotted curves) atoms below the critical temperature. (a) Temperature dependence at  $\mu = 10$ ,  $g = 0.1$ , and  $\omega = 2$ . (b) Interaction strength dependence at  $\mu = 10$ ,  $T = 3$ , and  $\omega = 2$ . (c) Chemical potential dependence at  $g = 0.1$ ,  $T = 3$ , and  $\omega = 2$ . (d) Potential frequency dependence at  $\mu = 10$ ,  $T = 3$ , and  $g = 0.1$ .

$r > r_1$ , the condensate density  $n_0(\mathbf{r}) = 0$ . The thermal density is determined by,

$$n_T(\mathbf{r}) = \sum_{k=1}^{\infty} \frac{e^{-k\beta[m\omega^2 r^2/2 + 2gn_T(\mathbf{r}) - \mu]}}{(\lambda_T \sqrt{k})^3}. \quad (12)$$

Whereas for  $r < r_1$ ,  $n_0(\mathbf{r}) \neq 0$ ,

$$n_T(\mathbf{r}) = \sum_{k=1}^{\infty} \frac{e^{k\beta[m\omega^2 r^2/2 + 2gn_T(\mathbf{r}) - \mu]}}{(\lambda_T \sqrt{k})^3}. \quad (13)$$

In Fig.1, we plot the various cases of the density profiles of condensed and noncondensed atoms in the spherically symmetric harmonic potential. Hereafter the units of  $\hbar = m = k_B = 1$  are used. For a better understanding of the dependence of the density on temperature, in Fig.2 we plot the total condensed atoms as a function of temperature. Figure 2(a) shows that the number of condensed atoms decreases with increase of interactions at a fixed chemical potential and a given temperature. Figure 2(b) is the number of condensed atoms for different chemical potentials at a given interaction. It coincides with the measurements carried out by Ensher et al[30]. In particular, as expected, it increases with the chemical potential.

We note that in our calculations that in our parameter ranges, the critical temperature is almost independent of the characteristic frequency  $\omega$  of the confining potential.

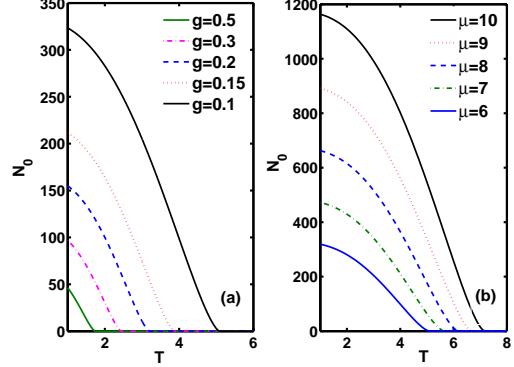


FIG. 2: (Color online) The condensed atoms versus the temperature for (a) various interaction strength at  $\omega = 1$  and  $\mu = 6$  and for (b) various chemical potentials at  $\omega = 1$  and  $g = 0.5$ .

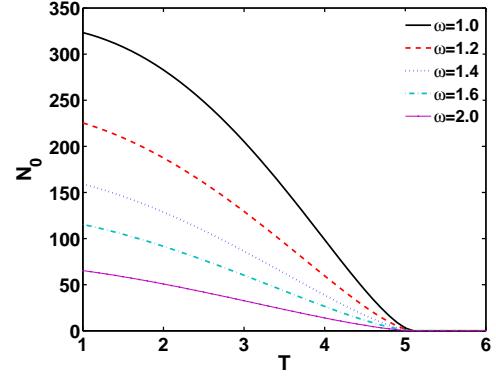


FIG. 3: (Color online) The condensed atoms versus the temperature for various frequencies of the confining potential at  $g = 0.1$  and  $\mu = 6$ .

Figure 3 reveals that all curves meet at one temperature point where the condensed atoms tend to zero. We consider that this result may be relevant to the mean-field theory when applying to a finite system, as well as semiclassical approximation in the calculation of the state density. Nevertheless, it implies that the condensation temperature is insensitive to the details of the confining trap.

At the critical temperature  $T_c$ , the condensed atoms is nearly zero. We obtain the critical temperature from Fig.2 for various interaction strength and chemical potentials, respectively, as shown in Fig.4. Figure 4(a) shows that the critical temperature  $T_c$  decreases with increase of the interaction strength  $g$ . The shift of critical temperature becomes saturated as the interactions increases. The inset is a log-log plot of the critical temperature versus the interaction strength. It reveals that the critical temperature decreases with the interaction strength or  $s$

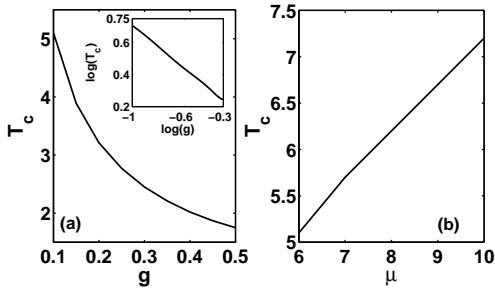


FIG. 4: (a) The critical temperature versus the interaction strength for  $\omega = 1$  and  $\mu = 6$ . Inset: The Log-Log plot gives a nearly linear relation with a slope  $\beta \approx -0.75$ . (b) The critical temperature versus the chemical potential for  $\omega = 1$  and  $g = 0.5$ .

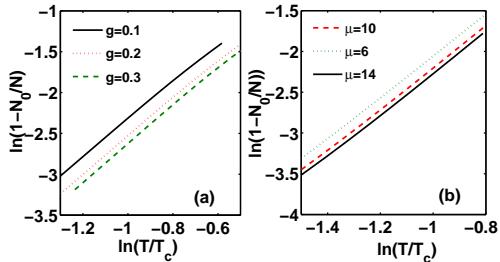


FIG. 5: (Color online) The log-log plot of the condensate fraction versus temperature for different interaction strength (a) and for different chemical potentials (b).

wave scattering length  $a_s$  as  $T_c \sim a_s^\beta$  with  $\beta \approx -0.75$ , in contrast to previous MFA calculations which give a linear relation  $\Delta T_c/T_c^{(0)} \approx -2.47 a_s n^{1/3}$  [12, 23]. Our results are qualitatively consistent with the experimental measurements by Smith et al [23]. Although the mean-field theory has weakness in dealing with the thermodynamical prop-

erties near the critical point, as discussed in Sec.II, it is remarkable that the results agree with the experiment quite well. Figure 4(b) shows that the critical temperature almost linearly increases with the chemical potential  $\mu$ .

To examine the universal behavior below the critical temperature, we study the temperature dependence of the condensate fraction  $N_0/N$  which takes the form,

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c}\right)^\gamma. \quad (14)$$

Figure 5 is a log-log plot of the condensate fraction versus the reduced temperature. It shows that for various interaction strength (Fig.5(a)) and chemical potentials (Fig.5(b)), respectively, the lines are parallel to each other, giving rise to a common slope  $\gamma \approx 2.3$ . This index  $\gamma$  is universal which is independent of the interaction strength, the chemical potential, as well as the frequency of the confining potential. In comparison, the ideal gas in a confining potential has an index  $\gamma_0 = 3$ , which is also independent of the characteristic frequency of the confining potential.

#### IV. SUMMARY

We have studied the thermodynamical properties of the interacting Bose gas confined in an external potential. For weak interactions, the system can be equivalent to an ideal gas in an effective mean-field potential where the eigenvalue of the generalized GP equation plays the role of the chemical potential. The critical temperature decreases nonlinearly with increase of interactions. Our results agree quite well with the recent experimental measurements. Furthermore, we found a universal relation of the condensate fraction with respect to the temperature below the critical temperature, with the index being independent of the interaction strength, the chemical potential, as well as the frequency of the confining potential. We expect verifications of the universal relation by experiments.

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